ABSTRACT OF THE DISCLOSURE

A computational method for the discovery and design of therapeutic compounds is provided. The methods used rely on an accurate inter-conversion of three-dimensional molecular spatial information between two alternative orthogonal representations. These methods enhance the accuracy for determining ab initio phases of macromolecular crystallographic structures at any desired experimental resolution limit. The computational technique employed utilizes a software program and associated algorithms. This method is an improvement over the current methods of drug discovery which often employs a random search through a large library of synthesized chemical compounds or protein molecules for bio-activity related to a specific therapeutic use. The development of computational methods for the prediction of specific molecular activity suggests a method for describing the contents of non-centro-symmetric sparsely packed crystals and the information provided therefrom will facilitate the design of novel chemotherapeutics or other chemically useful compounds.